Message

From: Washington, John [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=FDC3E8CE9F1D45C4894881FF420CA104-WASHINGTON, JOHN]
Sent: 6/10/2020 3:33:26 PM
To: Davis, Mary J. [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a11c3a4da6248dfbaecd3465fe1ebc3-Davis, Mary]
Subject: RE: Legacy Soil Core Data set
Attachments: 200609 JW NJ SoilCores_Targeted_MJBD_QA_200603_Weighted.xlsx

Hi Mary,

I finally finished my review – thanks for your patience.

Below I paste my latest suggestions, all minor and easy. See what you think. If you agree and address, I think this is ready to submit for clearance.

Great work as usual!
John

Pasted comments:

John's review 0n 200609 & 200610:					

Ex. 5 Deliberative Process (DP)

From: Davis, Mary J. <davis.maryj@epa.gov>
Sent: Tuesday, June 9, 2020 5:25 PM
To: Washington, John <Washington.John@epa.gov>
Subject: RE: Legacy Soil Core Data set

Hi John,

Ex. 5 Deliberative Process (DP)

I'll send you the ClPFPECAs file tomorrow morning once I get a chance to double-check the dups on the waters QQQ.

Thanks!

Mary

From: Washington, John <Washington.John@epa.gov>
Sent: Tuesday, June 9, 2020 4:23 PM
To: Davis, Mary J. <davis.maryj@epa.gov>
Subject: RE: Legacy Soil Core Data set

Hi Mary,

I reviewed your legacy PFAS Excel file on the soil cores and it all looks correct!

Ex. 5 Deliberative Process (DP)

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Considerations (as evaluated in attached Excel file-last worksheet):

Ex. 5 Deliberative Process (DP)

Thanks,
John

Pasted footnote from soils paper:

From: Davis, Mary J. <davis.maryj@epa.gov>
Sent: Thursday, June 4, 2020 9:09 AM
To: Washington, John <Washington.John@epa.gov>
Subject: RE: Legacy Soil Core Data set

Good morning, John!

I'm sorry that it's taken me so long to get this back to you. I've implemented your suggestion about weighting the in-vial concentrations, with a few modifications:

(1) I found, in practice, that it seemed to work best to multiply the in-vial concentrations by the ratio = (smallest rep mass)/(rep mass). This essentially reduces the larger sample mass concentrations in vials to reflect the actual concentration of the samples more accurately. This flipped ratio seemed non-intuitive to me at first, but I think it's essential because the actual concentration in the sample is calculated by dividing the concentration in the vial by the dry sample mass. This was done in the attached spreadsheet in "Sample_Conc Calcs_b" tab.

(2) As you mentioned, we probably want to do the more conservative approach to not over-represent differences between the samples and the process blanks. I found that this was achieved by the above method. To test this, I also multiplied in-vial concentrations by the ratio = (largest rep mass)/(rep mass), but I think this essentially increases the concentrations of the smaller sample masses. While this amounts to the same as the above approach with respect to sample rep variation, it causes a larger variation between the sample reps and the process blanks and thus shifts all samples to being more significant. Therefore, the above approach (1) is preferred. This calculation was done in the "Sample_Conc Calcs_c" tab.

(3) In both of the above tabs, I determined the significance/color coding based on the weighted concentrations in vials, but in the last section (furthest right) I copied the values of concentrations in samples directly from the "Sample_Conc Calcs" tab. So, the colors reflect weighted methods, but the final concentrations are calculated normally. Essentially, you can look at the unweighted, weighted small, and weighted large effects on the color coding by comparing the rightmost matrix in each tab.

Ex. 5 Deliberative Process (DP)

This is probably better to discuss over the phone. I'm generally available today outside of the CPSB checkin and the 1:30 webinar.

I'd plan to do this same thing with the ClPFPECA data set, but wanted to check the method with you beforehand.

Thanks,

Mary

From: Washington, John <Washington.John@epa.gov>
Sent: Tuesday, June 2, 2020 11:04 AM
To: Davis, Mary J. <davis.maryj@epa.gov>
Subject: RE: Legacy Soil Core Data set

Here is a brainstorming thought:

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Just a thought . . .

From: Washington, John
Sent: Tuesday, June 2, 2020 10:51 AM
To: Davis, Mary J. <davis.maryj@epa.gov>
Subject: RE: Legacy Soil Core Data set

OK, a fair concern. Remembering our objective is to achieve the best approximation of reality, I suggest you try both ways so we can inspect whether we arrive at different conclusions on one or more analytes, and, if we do, then we can reason thru together what is most justifiable.

On the plus side, 1) often we are looking at order-of-magnitude differences, samples to blanks, so 2-fold variation from weight in samples might not compromise our detection of differences when differences are present; and 2) high values (and pragmatically more consequential in some respects) should differ from blanks regardless of 2-fold sample weight variation. On the down-side, a statistical loss of a few low values might detract considerably from us finding patterns.

From: Davis, Mary J. <davis.maryj@epa.gov>
Sent: Tuesday, June 2, 2020 10:37 AM
To: Washington, John <Washington.John@epa.gov>
Subject: RE: Legacy Soil Core Data set

Hi John,

Thanks… though again, I think having such a large variation in dry mass used to create sample replicates should be addressed. I don't think that the variation of a given sample should be reported as being super high if it's only because of the significant difference in dry mass. Two replicates might look very different based on their concentrations in the vial, but then when you calculate the concentration in the sample, they're very similar. The opposite could also be true (similar concentrations in vial, but different concentrations in the sample). This hasn't been an issue for other sample sets I think because the dry sample masses were very close between replicates. I'm not sure why these are so different.

Maybe I'm missing something…

Mary

From: Washington, John <Washington.John@epa.gov>
Sent: Tuesday, June 2, 2020 10:30 AM
To: Davis, Mary J. <davis.maryj@epa.gov>
Subject: RE: Legacy Soil Core Data set

Yes Mary,

I agree it is best to calculate difference from blanks based on analytical values of the vial extracts that went on the instrument. In general this is the better approach I think . . . apples to apples. And I think it is best to leave the field blank out of the LOQ evaluation -- field blanks test for additional sources of variation. While any single field blank might look like process blanks, if we exclude them as a rule from LOQ calcs, then when we encounter a high field blank we have less explaining to do.

By the way, Chris emailed me that he will not make today's meeting – he didn't say why. Maybe if Brad can't answer your LC-method questions, you or we could set up a call with Chris.

Good email back from Sandra!

John

From: Davis, Mary J. <davis.maryj@epa.gov>
Sent: Tuesday, June 2, 2020 10:20 AM
To: Washington, John <Washington.John@epa.gov>
Subject: RE: Legacy Soil Core Data set

Hi John,

It's a good thing you hadn't gotten to the data yet… I keep finding things. For example, the latest is that I originally included the field blank along with the process blanks in evaluating LOQ (my thought being that you probably also want the samples to be significant with respect to the field blank)… but looking at your old legacy data sets, I'll just use the Field blank in QA instead.

I do have a question though. In the deep soils, it looks like the sample masses used in the extractions vary a decent amount between sample reps (eg. sample 1.2 used 1.67g dry sample weight while 1.3 used 2.52g sample; sample 2.1 used 1.77g sample while sample 2.3 used 2.97g sample)… this would obviously lead to variation in the concentration in the vials that isn't necessarily reflective of variation in the samples.

As you know, the significance of the concentrations is determined using the concentration in the vials… but given the large variation in dry mass sample used, I'm wondering if it would be better to compute statistics based on the sample concentration? At least for the soil cores.

What are your thoughts?

Thanks!

Mary

From: Washington, John <Washington.John@epa.gov>
Sent: Monday, June 1, 2020 9:03 AM
To: Davis, Mary J. <davis.maryj@epa.gov>
Subject: RE: Legacy Soil Core Data set

Haha Mary, I am replying to your last email. If that's the worst slip you ever do, you will have had a fantastic run.

I haven't had a chance to look at the data yet, sorry. I plan to this week.

From: Davis, Mary J. <davis.maryj@epa.gov>
Sent: Monday, June 1, 2020 8:59 AM
To: Washington, John <Washington.John@epa.gov>
Subject: RE: Legacy Soil Core Data set

Good morning, John!

I apologize for sending all these emails your way this morning. Upon double-checking, I realized that I forgot to subtract process blank concentrations from these legacy concentration values ☹ That was dumb, sorry! I was in part using my previous QA-submitted ClPFPECA Veg file as a model, and process blanks weren't an issue there. I'll work on updating that this morning, but did you find anything else that I should correct while I'm at it?

Thanks,

Mary

From: Davis, Mary J.
Sent: Wednesday, May 27, 2020 4:12 PM
To: Washington, John <Washington.John@epa.gov>
Subject: Legacy Soil Core Data set

Hi John!

I've attached the legacy soil core data set for your review. Please let me know what you think might need editing. Of particular note, I did have peaks in a couple of the solvent blans, but I tried to explain them on the spreadsheet. I wasn't sure what the best way to handle them would be.

Working on cleaning up the ClPFPECA Soil Cores now.

Thanks,

Mary

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